Development of Interface-Dislocation Dynamics Simulations for Nanoscale Metallic Composites

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Extensive investigations over the past decade indicate that nanoscale metallic composites have unprecedented levels of strength, ductility, and damage tolerance in extreme environments. However, the current meso-/macro-scale materials modeling cannot predict the mechanical response of such nanoscale composites because they do not account for the role of the interface mechanical deformation. In this work, we apply findings from atomistic simulations to develop an Interface-Dislocation Dynamics (DD) simulation code with the focus on capturing the fundamental physics of dislocation-interface interactions, such as annihilation, nucleation, and emission within, at, and across the interface. With this model, we can study the influence of interface structure and properties and the misorientation on the development of plastic deformation in nanoscale composites. These findings will enable the development of material modeling tools at continuum-length scales.

Multilayered materials, typically synthesized by physical vapor deposition or electro-deposition techniques, exhibit significant increases in strength as the layer thickness is decreased from the micrometer to nanometer scale [1]. It has been widely recognized that materials properties can be significantly improved or degraded by virtue of interface structures [2]. Atomic-scale modeling is able to reveal the unit process (involving single or a few defects) during deformation with respect to kinetics and energetics, but is limited to timescale (ns) and lengthscale (nm) [3]. Current state-of-the-art continuum modeling can only treat interface boundaries phenomenologically without any structural characteristics [4]. For materials containing high-density interfaces, it is still a challenge in incorporating interface physics, such as nucleation, motion, reactions, etc., in current models. The bottleneck is attributed to three reasons: (1) lack of knowledge of interface-dominated deformation mechanisms, in particular of dislocation-interface interactions; (2) slips in the adjacent grains are not directly correlated to the interface with respect to their orientation relations, interface structures, and interface properties; and (3) a generic interface model representing the structure and properties of interfaces does not exist.

DD simulations, in which dislocations are the simulated entities, offer a way to extend length and time scales beyond those of atomistic simulations, and have the unique advantage of exploring dislocation activities [5] due to (1) the powerful capability of modeling the behavior of metallic materials at the micro-scale in a more physical manner than existing continuum plasticity models, and (2) direct observation of dislocation activities in simulated samples. In most studies, DD simulations have been implemented on single-crystal materials, such as investigations of strain hardening of bulk materials under low and high strain rates [6], dislocation motions and interactions in thin films [7], and size-dependent plasticity of single-crystal nano-/micro-pillars [8]. In this work, by combining atomistic studies with DD simulation, we developed an Interface-DD model for metal-metal interfaces to overcome the weakest areas in the DD simulations–in accounting for the special roles of interfaces on storage, recovery, nucleation, and emission of dislocations within, at, and across interfaces. The development of the interface-DD model relies heavily on the understanding of dislocation-interface interaction at atomic scale.

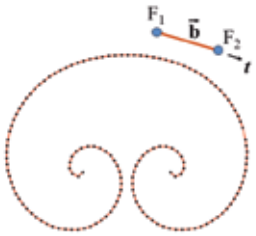

Fig.1. Illustration of the discretization of a Frank-Read dislocation source in 3D DD simulations.

In 3D discrete DD simulations, dislocations are discretized into segments, as shown in Fig. 1. Each segment contains the information of dislocations, such as Burgers vector, line direction, forces, and mobility. The total force on each segment is calculated by the Peach–Koehler (PK) equation:

$$\mathbf{F}_{PK} = \left(\left(\alpha_{app} + \sigma_{int}\right)\cdot \mathbf{b}\right)\times \mathbf{t} + \mathbf{F}_{self} \quad (1)$$

where σ_{app} is the applied stress tensor, σ_{int} is the stress tensor from the other defects, $\boldsymbol{b}$ is the Burgers vector of the dislocation, $\boldsymbol{t}$ is the line direction of a given segment, and $\mathbf{F}_{\text{self}}$ is the self-force of the dislocation segment.

During the deformation, the plastic strain rate is obtained from the motion of dislocations as

$$\dot{\varepsilon}^{p} = \frac{1}{2V}\sum_{i=1}^{N_{tot}} l_i^{\alpha} v_i^{\alpha}\left(\mathrm{b}_i \otimes \mathrm{n}^{\alpha} + \mathrm{n}^{\alpha} \otimes \mathrm{b}_i\right) \quad (2)$$

where V is the volume of the simulated crystal, N_{tot} is the total number of dislocation segments, l_i^{α} is the length of dislocation segment i moving on the slip plane α, and v_i^{α} is the corresponding moving velocity of the segment i. $\boldsymbol{b}_i$ and $\boldsymbol{n}^{\alpha}$ are the Burgers vector of dislocation segment i and the normal of slip plane α, respectively.

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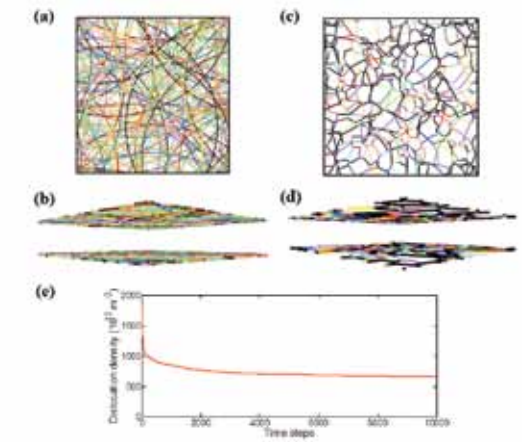

Fig. 2. (a) Top view of initial dislocation structure for bilayer Cu/Nb system, (b) side view of (a), (c) top view of relaxed dislocation structure for bilayer Cu/Nb system, (d) side view of (c), and (e) the evolution of dislocation density during relaxation.

Atomistic simulations so far reveal that (1) interface sliding can be represented as a result of the nucleation and glide of glide-type interfacial dislocations, (2) lattice dislocations can nucleate from interfaces [9], (3) all types of interfacial dislocations can move through either glide or climb, and (4) once lattice dislocation enters interfaces, it becomes an interfacial dislocation (conserves the Burgers vector but loses the slip plane). As a consequence, it moves along the interface through either climb or glide, and acts as sources for nucleating lattice dislocation. In keeping with these findings, we develop the rules of the nucleation and reaction of interfacial and lattice dislocations in the interface-DD model.

With the dislocation-interface interaction rules developed in our DD-interface model, we studied the mechanical response of a Cu/Nb bilayer system under external load. Initially, dislocation loops were generated in both and the Burgers vectors for these loops were randomly chosen from Burgers vectors in both Cu and Nb phases as shown in Fig. 2(a-b). Then the system was relaxed to equilibrate the dislocation microstructure. Figures 2(b-c) and (d) show the final equilibrated dislocation structure and the evolution of the dislocation density during relaxation, respectively. After relaxation, an external load much like that in the experiment was applied on the system. Driven by the external load, lattice dislocations nucleated from the interface to accommodate the applied deformation. After nucleation, lattice dislocations continued propagating in phases due to the operation of Frank-Read sources. Once approaching another interface, the front part of the half dislocation loop was absorbed by the interface and two threading dislocations were formed after the front part of the dislocation loop was truncated by the interface. Under external load, these two threading dislocations propagated in the Cu phase and generated plastic strain to minimize the internal strain energy. Figure 3 (a) shows one example of the whole process of the nucleation of lattice dislocations from interfaces and the propagation of threading dislocations in the Cu phase. With increasing load, lattice dislocations continued nucleating from the interface and generated large amounts of plastic deformation in the system. Figure 3 (b) shows the dislocation structure of the deformed system at 2% total strain.

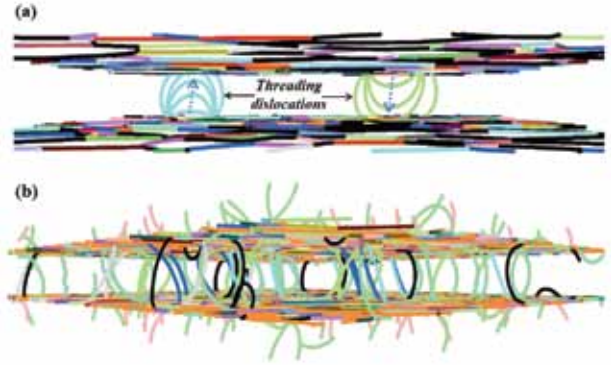

Fig. 3. (a) Progress of lattice dislocations nucleating from interfaces and the formation of threading dislocations after nucleated dislocations absorbed by the interface (dashed arrows indicate dislocation operating direction), (b) plot of dislocation structure after deformation at 2% total strain.

In this work, we developed a DD simulation model based on observations from atomic-scale simulations and experimented to study the dislocation-interface interactions at micro- and nano-scales, and provide a generic bi-metal interface model that represents the key characteristics of the structure and properties of the interface. This model can also be applied to dislocation interactions with grain boundaries and twin boundaries, since the basic physical processes such as dislocation absorption, nucleation and transmission from interfaces are the same. Our improvement on current DD simulations removes the restriction on single-phase materials and fills the gap in materials modeling on interface problems between atomic-scale models and continuum plasticity models.

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